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Abstract

New approaches are being developed to facilitate multidisciplinary collaborative research of Homogenous Charge Compression Ignition (HCCI) combustion processes. In this paper, collaborative sharing of the Range Identification and Optimization Toolkit (RIOT) and related data and models is discussed. RIOT is a developmental approach to reduce the computational complexity of detailed chemical kinetic mechanisms, enabling their use in modeling kinetically-controlled combustion applications such as HCCI. These approaches are being developed and piloted as a part of the Collaboratory for Multiscale Chemical Sciences (CMCS) project. The capabilities of the RIOT code are shared through a portlet in the CMCS portal that allows easy specification and processing of RIOT inputs, remote execution of RIOT, tracking of data pedigree and translation of RIOT outputs (such as the reduced model) to a table view and to the commonly-used CHEMKIN mechanism format. The reduced model is thus immediately ready to be used for more efficient simulation of the chemically reacting system of interest. This effort is motivated by the need to improve computational efficiency in modeling HCCI systems. Preliminary use of the web service to obtain reduced models for this application has yielded computational speedup factors of up to 20 as presented in this paper.

Keywords: HCCI, mechanism reduction, informatics, collaboration, web portal

1. Introduction

Homogeneous charge, compression ignition (HCCI) is a piston-engine combustion process that has emerged as a high-efficiency alternative to traditional spark-ignition (SI) combustion and a low-emissions alternative to traditional diesel combustion. It offers good fuel economy, similar to a diesel engine, while producing very low emissions of NO_x and soot particulate matter. However, before HCCI can be implemented in production engines, several technical barriers must be overcome. Research and development are being pursued in a number of areas, including: control of ignition timing over the load/speed map, slowing the heat-release rate at higher loads, controlling hydrocarbon and carbon monoxide emissions, maintaining combustion stability, cold starting, and response to load and speed transients.

Computer modeling of the in-cylinder processes in an HCCI engine is a key element in this research and development effort. Modeling methodologies for HCCI range from adiabatic single-zone models (cf. [1]) to integrated multi-dimensional CFD/kinetics engine models (cf. [2]). Due to the nature of HCCI, the ignition, combustion heat-release and pollutant formation processes are much more highly coupled to the chemical kinetics of the charge mixture than they are for traditional SI or diesel combustion. Therefore, the usefulness of HCCI modeling results relies heavily on the accuracy of the chemical-kinetics mechanism employed and its ability to match the behavior of the specific fuel in use. For a limited number of reference fuels, detailed kinetic mechanisms have been developed [3,4] and have provided useful understanding of the in-cylinder processes [2].

However, these detailed mechanisms often contain many hundreds of species and thousands of reactions and their direct implementation in HCCI modeling can result in

computational times that are impractical. As new tools are developed for constructing more detailed mechanisms, the computational expense of modeling reaction kinetics using these mechanisms will only increase. Thus, there is clearly a need for new approaches to improve the computational efficiency of using the mechanisms while preserving the level of chemical detail. Such an approach would substantially improve our ability to simulate HCCI combustion, and therefore, provide a valuable component in overcoming the technical barriers to HCCI.

1.1 Enabling HCCI Science with New Tools and Approaches

A more efficient combination of multi-dimensional CFD and chemical-kinetics modeling is required to facilitate research, for example, on the effects of non-uniformities in the charge mixture and temperature in HCCI. We are exploring, therefore, the adaptation of detailed reaction mechanisms to specific conditions or sub-problems to enable their reduction to a more tractable size without sacrificing the ability to capture the important chemistry of the conditions studied. Individual zones in a combustion chamber experience a smaller range of conditions than the entire combustion chamber as illustrated in Fig. 1 depicting the computational domain for an HCCI simulation. The idea is to then reduce the kinetic model to a much smaller subset that is still accurate over each zone to which it is applied. This approach requires access to new developmental tools and ways for researchers to efficiently manage the process of model reduction and the associated proliferation of data and metadata. These researchers are collaborating from multiple disciplines and locations, and must be able to work together efficiently with developmental tools and evolving data. The RIOT web service for automatic

reaction mechanism reduction was developed as part of the Collaboratory for Multiscale Chemical Science (CMCS) to accomplish this goal, as discussed in the next section.

More about the vision of CMCS and its informatics infrastructure can be found in a recent paper [5] and on the CMCS web site (cmcs.org).

2. The RIOT/CMCS Web Service

2.1 Overview

RIOT (Range Identification and Optimization Toolkit) is a software tool that is being developed to allow reduction of the number of reactions in a reaction mechanism while maintaining user-specified tolerances on the accuracy of the reduced mechanism [3,4]. The basic idea is to reduce the model without significantly changing the predictions of values such as temperature, pressure and species compositions, relative to the full model. CMCS has integrated the RIOT model reduction code into its portal environment by developing a portlet interface that assists the user with specifying inputs to the RIOT code, generates the input file, ships the request to a web service interface to the code, and uploads and presents the results when the reduction completes.

2.2 Using the RIOT Portal to Reduce a Mechanism

The RIOT program requires several input files to perform the mechanism reduction. These files include a detailed chemical kinetic mechanism file, a thermodynamics data file and one or more solution data files. The first two files are assumed to be in CHEMKIN format [6]. The solution data files contain histories of pressure, temperature, and species compositions, representative of the set of reaction conditions for which the reduced model will be used. For HCCI, this would likely be computed histories from a simulation of an HCCI ignition in an engine.

Once the user has assembled the required files, the user uploads them to the portal using the Data Browser portlet. The portal recognizes the reaction mechanism file and the thermodynamic data file based on their MIME-types (".mech" and ".therm" respectively). The user then accesses the RIOT portlet and specifies the set of files to be used for the reduction. One or more solution data files can be specified. Multiple data files may be needed to cover a broad range of conditions (pressure, temperature, fuel composition, equivalence ratio and exhaust gas recirculation) for HCCI.

In the RIOT portlet, the user selects the solution data points to be considered in reducing the model and specifies the tolerances that affect the accuracy of the model. The user selects the points that have the critical temperatures and pressures where the reduced mechanism should be valid. A "Model Reduction Parameters" button provides access to a portlet page where error tolerances are specified for the model reduction. The user then presses a "submit" button to reduce the mechanism. The mechanism and all required inputs are sent via an asynchronous web-based service to a server at MIT where the mechanism reduction is performed. When the calculation is finished, an XML-based reduced mechanism file is returned to the CMCS data store where it is available in the RIOT portlet. When the entire process completes, the user receives an email notification with a link that leads directly to the file in the portal. Within the portal, the XML-formatted results file can be easily translated to a table view, or to a CHEMKIN-format file, etc., for use with desired reacting process simulators.

The portal provides a graph that allows a user to track the pedigree of the reduced model. The user can trace the reduced model back to the detailed model and the specified

conditions that were used to create it, enabling users to follow the pedigree of the data without having to contact other scientists who created the data.

3. Case Study: HCCI modeling facilitated by RIOT/CMCS web service

To demonstrate the potential impact of this application, the RIOT tool on CMCS was used to reduce a mechanism for modeling HCCI using iso-octane fuel at the conditions summarized on Table 1. The full detailed kinetic model used was the LLNL mechanism [4] with 857 species participating in 3606 reactions. A single-zone HCCI simulation was performed first using the full mechanism and it was completed after 2280 seconds of CPU time.

In the manner described in the previous section, a ready-to-use reduced model was obtained, consisting of 660 reactions with only 257 participating species (viewable at [7]). The simulation was then repeated using this reduced model and the computation required only 111 seconds of CPU time – a decrease by a factor greater than 20. Comparisons of the Temperature and Pressure histories predicted by the full model and the reduced model also show that the reduced model was very accurate (see Figs. 2 and 3).

4. Conclusions

Collaborative sharing of RIOT for automatic reaction mechanism reduction and related data for enabling HCCI modeling has been discussed. RIOT has been integrated into the CMCS portal environment through development of a portlet interface that assists the user with specifying inputs to the RIOT code, generates the input file, ships the request to a web service interface to the code, and uploads and presents the results when the reduction completes. Preliminary use of the RIOT/CMCS web service to obtain a

reduced model for modeling HCCI yielded greater than a 20-fold improvement in computational efficiency while preserving the accuracy of the predictions. We plan to continue development and improvement of the RIOT tool and associated CMCS capabilities for HCCI engine applications.

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Table 1

Input parameters for HCCI engine simulation

| Parameter | Value |
|---|--------------|
| Pressure (atm) | 0.9776 |
| Temperature (K) | 402 |
| Engine Compression Ratio | 15.9 |
| Engine Connecting Rod to Crank Radius Ratio | 3.2 |
| Engine Speed (rpm) | 1200 |
| Iso-octane (mole fraction) | 0.00612 |
| Oxygen (mole fraction) | 0.20823 |
| Nitrogen (mole fraction) | 0.78565 |

List of Figure Captions

Figure 1: An expanded view of a model HCCI engine combustion chamber divided up into zones (indicated by color) so that each can be assigned a different chemical model by the Range Identification and Optimization Toolkit. (Figure courtesy D. L. Flowers, LLNL).

Figure 2: Comparison of Temperature profiles using RIOT reduced mechanism and full detailed mechanism.

Figure 3: Comparison of Temperature profiles using RIOT reduced mechanism and full detailed mechanism.

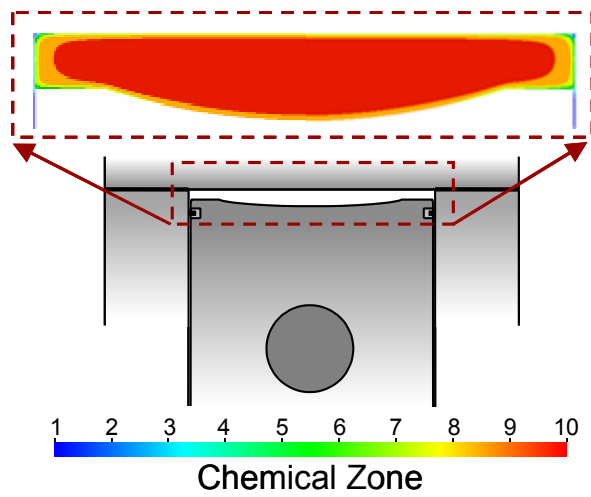


Figure 1.

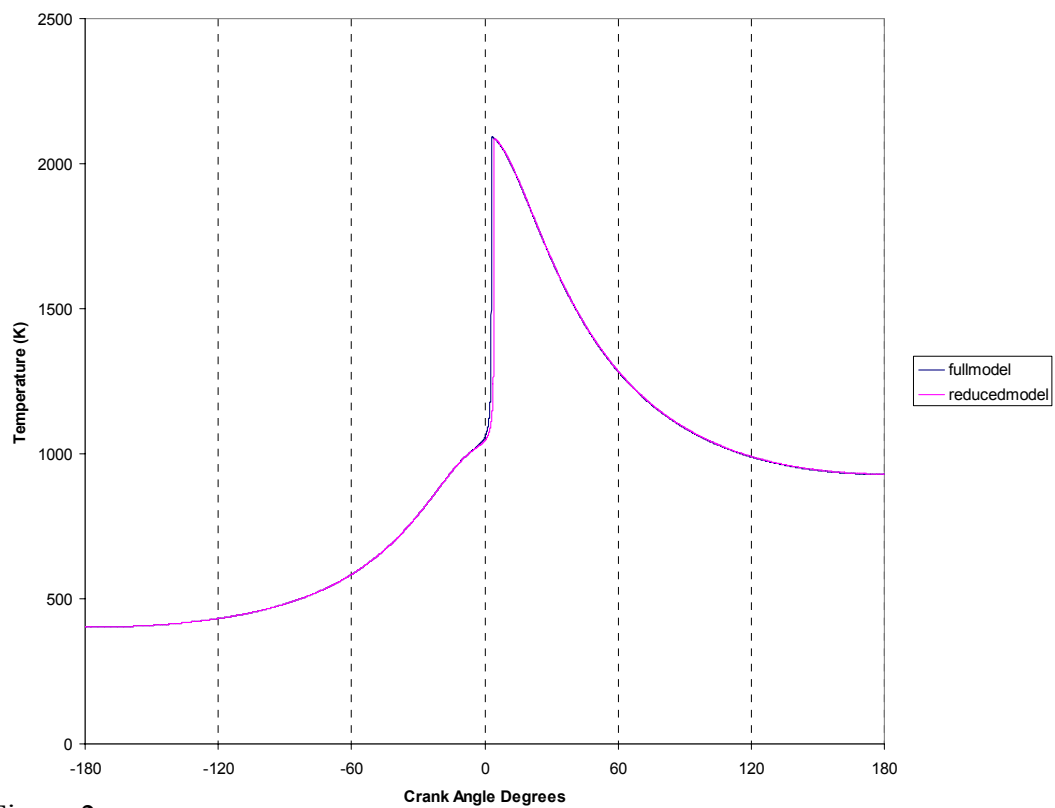


Figure 2.

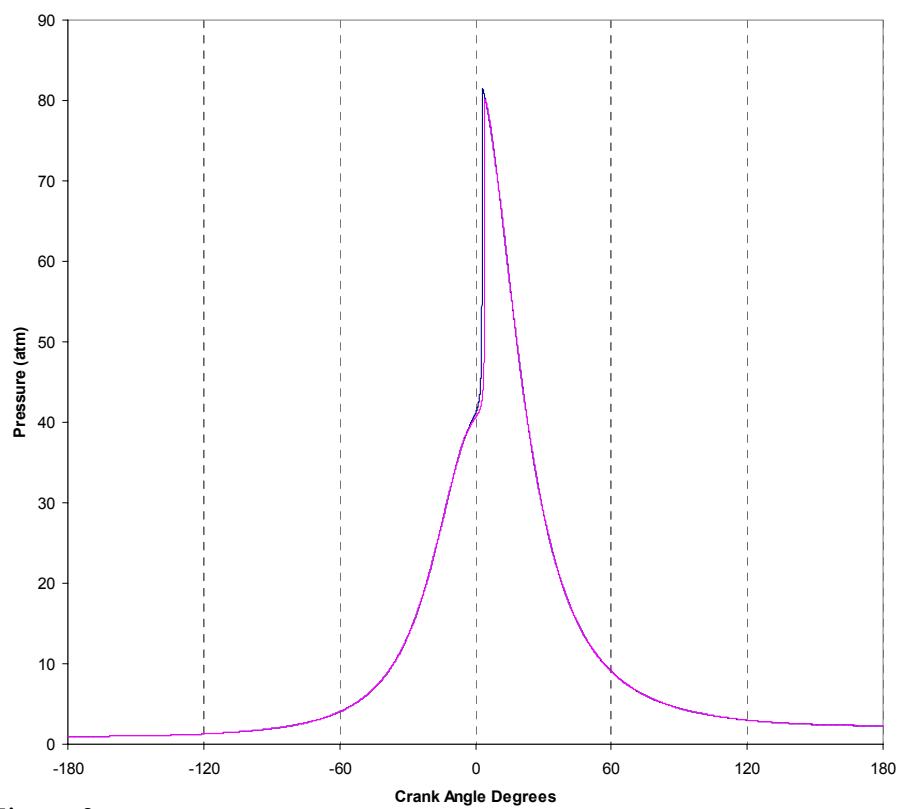


Figure 3.